DEPARTMENT OF CHEMISTRY
COLLEGE OF ARTS AND SCIENCES

SUMMER RESEARCH OPPORTUNITIES FOR UNDERGRADUATE WOMEN

FOR APPLICATION YEAR: 2021

PROJECT TITLE: Data science modeling of the dynamics of protein complexes

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Project Description

Research in the Dima group focuses on understanding the role of various structural and cellular factors in the mechanical response of biological molecules ranging from small RNA molecules and multi-domain proteins to large fibrillar assemblies that play crucial roles in fundamental processes such as the maintenance of the cell shape, cell mobility, cell-cell adhesion, axonal growth, and cellular division (mitosis).
A project for a WISE student is â€œData science modeling of the dynamics of protein complexes". Microtubules, large multi-filament polymeric complexes which are the main component of the cell cytoskeleton, play fundamental roles in cellular processes ranging from cellular transport to mitosis. These roles are all intimately connected with microtubules' ability to depolymerize under controlled cellular conditions. This control is exerted by a large array of molecular machines (300 or so species), which form transitory complexes with microtubules over different timescales. Recent experimental results strongly suggest that these protein cofactors work by converting chemical energy into mechanical work, which is then applied to the microtubule polymer lattice, but little is known about the details of the process. The goal of this project is to determine the relationship between the steps in the working cycle of such molecular machines and the structural changes taking place inside the protein subunits of the machines and of their substrates, which are important during processes such as mitosis or cell-cell adhesion.
The WISE student will gain experience with (1) data science (machine learning) methods in chemistry, (2) simulation software designed to follow protein structure deformation under applied forces, and (3) data analysis that couples results of simulations with experimentally derived data.